

The virial theorem and the method of multipliers in spectral theory

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Abstract

We provide a link between the virial theorem in quantum mechanics and the method of multipliers in theory of partial differential equations. After giving a physical insight into the techniques, we show how to use them to deduce the absence of eigenvalues and other spectral properties for electromagnetic Schrödinger operators. We focus on our recent developments in non-self-adjoint settings, namely on Schrödinger operators with matrix-valued potentials, relativistic operators of Pauli and Dirac types, and complex Robin boundary conditions.

Keywords: virial theorem, method of multipliers, absence of eigenvalues, uniform resolvent estimates, electromagnetic Schrödinger and Dirac operators, non-self-adjoint perturbations, Robin boundary conditions

1 Quantum-mechanical background

In quantum mechanics, physical states and observables are represented by vectors and self-adjoint operators in a Hilbert space \mathcal{H} , respectively. The expectation value of an observable A to be in a state Ψ is given by the inner product $\langle A \rangle := (\Psi, A\Psi)$ and the outcomes of measuring are the spectrum of A . The most prominent observable is the Hamiltonian H representing the total energy of the system. It determines the evolution of states in time t through the Schrödinger equation

$$i \frac{d\Psi}{dt} = H\Psi. \quad (1)$$

The eigenvalues λ of H are energies of the system for which (1) admits stationary solutions of the type $e^{-i\lambda t}\psi$, where ψ is an eigenvector of H corresponding to λ ; it is customarily called a *bound state* (or *trapped mode*). The exclusion of eigenvalues constitutes a first step in justifying transport for a quantum system.

2 The virial theorem

How to achieve the absence of eigenvalues of a given operator H ? A powerful tool is represented by an abstract version of the *virial theorem* (see [10, Sec. 13 & Notes] for a historical background). Let us present a formal statement first.

Let T be another self-adjoint operator in \mathcal{H} . Assume that the commutator of T with H is *positive* in a sense. For instance, in a very restrictive sense, that there exists a positive number a such that (we do not care about operator domains for a moment)

$$i[H, T] \geq aI \quad (2)$$

in the sense of quadratic forms in \mathcal{H} .

Now, let λ be an eigenvalue of H corresponding to an eigenvector ψ , normalised to 1 in \mathcal{H} . That is, the stationary Schrödinger equation

$$H\psi = \lambda\psi \quad (3)$$

holds. Then we get a contradiction

$$\begin{aligned} a &\leq (\psi, i[H, T]\psi) \\ &= i(H\psi, T\psi) - i(T\psi, H\psi) \\ &= i(\lambda\psi, T\psi) - i(T\psi, \lambda\psi) \\ &= 0, \end{aligned} \quad (4)$$

where the first and last equalities employ the self-adjointness of H and T . Note that our convention is that the inner product (\cdot, \cdot) of \mathcal{H} is linear in the second component.

Hence, the positivity of the commutator prevents the existence of eigenvalues. This is the formal statement of the virial theorem. Schematically:

$$\text{positivity (2)} \implies \sigma_p(H) = \emptyset,$$

where $\sigma_p(H)$ denotes the point spectrum of H , i.e. the set of eigenvalues.

3 The method of multipliers

The virial theorem is closely related with the *method of multipliers*, usually attributed to the original development of Morawetz [9].

Take an inner product of both sides of (3) with the vector $\phi := iT\psi$ (this is the multiplier of the method) and take twice the real part of the obtained identity:

$$\begin{aligned} (\psi, i[H, T]\psi) &= (iT\psi, H\psi) + (H\psi, iT\psi) \\ &= 2\Re(\phi, H\psi) \\ &\stackrel{\downarrow}{=} \lambda 2\Re(\phi, \psi) \\ &= \lambda [(iT\psi, \psi) + (\psi, iT\psi)] \\ &= 0 \end{aligned}$$

(here the arrow points to the initial identity, the other equalities are manipulations). In this way we have arrived at the same identity as in (4) and the same contradiction under the positivity hypothesis (2).

4 An evolution interpretation

Why the positivity of the commutator is related to the (total) absence of eigenvalues? How to choose the auxiliary (so-called *conjugate*) operator T ? It is useful to get a physical insight first.

Differentiating the expectation value of T with respect to time t and using (1), we (formally) get

$$\begin{aligned} \frac{d\langle T \rangle}{dt} &= \left(\frac{d\Psi}{dt}, T\Psi \right) + \left(\Psi, T \frac{d\Psi}{dt} \right) \\ &= (-iH\Psi, T\Psi) + (\Psi, T(-iH\Psi)) \\ &= i(\Psi, HT\Psi) - i(\Psi, TH\Psi) \\ &= (\Psi, i[H, T]\Psi) \\ &= \langle i[H, T] \rangle. \end{aligned} \quad (5)$$

Hence the evolution of the expectation value of T is given by the expectation value of the commutator with H multiplied by i (without this multiplication, the commutator $[H, T]$ is actually skew-adjoint).

It follows from (5) and (2) that the differential inequality

$$\frac{d\langle T \rangle}{dt} > a$$

holds (assuming the normalisation $\|\Psi\| = 1$), which in turn implies

$$\langle T \rangle(t) > \langle T \rangle(0) + at$$

for all times $t \geq 0$. Consequently,

$$\lim_{t \rightarrow +\infty} \langle T \rangle(t) = +\infty. \quad (6)$$

In summary, the positivity of the commutator (2) implies that the expectation value of T diverges.

5 The free Hamiltonian

To answer the pertinent questions at the beginning of Section 4, let us focus on the Hamiltonian of a free (i.e. no forces) non-relativistic (i.e. no spin) particle. It is customarily represented by the operator

$$H_0 := -\Delta \quad \text{in} \quad L^2(\mathbb{R}^d), \quad (7)$$

which is self-adjoint provided its domain is chosen to be the Sobolev space $W^{2,2}(\mathbb{R}^d)$. Note that $H_0 = P_0^2 := P_0 \cdot P_0$, where the dot denotes the scalar product in \mathbb{R}^d and $P_0 := -i\nabla$, with domain being the Sobolev space $W^{1,2}(\mathbb{R}^d)$, represents the momentum of the particle. In this representation, the position of the particle is represented by the maximal operator of multiplication X by the space variable x , i.e. $X\psi(x) = x\psi(x)$.

Now, let T_0 be the quantum counterpart of the radial momentum of the particle:

$$T_0 := \frac{X \cdot P_0 + P_0 \cdot X}{2} = -ix \cdot \nabla - i\frac{d}{2}. \quad (8)$$

Note that we had to take a symmetrised version of the classical radial momentum $X \cdot P_0$ (in order to make T_0 self-adjoint, at least formally), since the observables X and P_0 do not commute in quantum mechanics. Then (6) can be interpreted in physical terms as that the particle escapes to infinity of \mathbb{R}^d for large times (for the radial derivative diverges). That is, the particle is not bound, it propagates. More specifically, the stationary solutions of the Schrödinger equation (1), corresponding to initial data being eigenfunctions, do not exist.

It remains to analyse the validity of (2) for the free Hamiltonian (7) and the radial momentum (8). It is easily verified that (still formally)

$$i[H_0, T_0] = 2H_0.$$

Here the right-hand side is non-negative because, by an integration by parts,

$$(\phi, H_0\phi) = (\phi, -\Delta\phi) = \|\nabla\phi\|^2 \geq 0 \quad (9)$$

for every $\phi \in W^{2,2}(\mathbb{R}^d)$. However, it is not positive in the strict sense (2) for $\sigma(H_0) = [0, \infty)$. Nonetheless, a contradiction in the spirit of (4) is still in order:

$$\begin{aligned} 2 \|\nabla \psi\|^2 &= (\psi, 2H_0 \psi) \\ &\stackrel{\downarrow}{=} (\psi, i[H_0, T_0] \psi) \\ &= 0, \end{aligned} \quad (10)$$

whenever ψ is an eigenfunction of H_0 . Indeed, from this identity we deduce that ψ is constant, which is not possible for a non-trivial function in $L^2(\mathbb{R}^d)$.

In summary, commutators arise in evolution processes in quantum mechanics and the natural choice for the conjugate operator for the free Hamiltonian H_0 is given by the radial momentum (8).

6 Dispersion

There is yet another support for the choice (8), at least if we deal with the Laplacian and its perturbations. In fact, the conjugate operator T_0 by itself arises as a commutator with the Laplacian:

$$T_0 = i \left[H_0, \frac{X^2}{4} \right].$$

Consequently,

$$\frac{d^2}{dt^2} \left\langle \frac{X^2}{4} \right\rangle = \frac{d}{dt} \langle T_0 \rangle = \langle i[H_0, T_0] \rangle,$$

so the positivity of the commutator $i[H_0, T_0]$ actually shows that the expectation value of the square of the magnitude of the position is a convex function in time: there is a *dispersion*.

7 Rigorous implementation

There are certainly a number of formal manipulations in the arguments given above. Let us now show how to justify them for the free Hamiltonian.

The eigenvalue equation (3) for the free Hamiltonian precisely means that there exists a non-trivial function $\psi \in W^{2,2}(\mathbb{R}^d)$ such that

$$(\nabla \phi, \nabla \psi) = \lambda (\phi, \psi). \quad (11)$$

for any choice $\phi \in W^{1,2}(\mathbb{R}^d)$. This is just a weak formulation of the Helmholtz equation in \mathbb{R}^d .

First of all, notice that we may restrict to $\lambda \geq 0$ due to the self-adjointness of H_0 and (9).

In other words, the existence of non-real and negative eigenvalues is easily disproved.

Following the arguments given above, our aim is to choose $iT_0\psi$ for the test function (the multiplier) ϕ , where the conjugate operator T_0 is given by (8). However, it is not clear that ψ belongs to the domain of T_0 (the domain of T_0 has not been even discussed) and, even if so, that $\phi \in W^{1,2}(\mathbb{R}^d)$. Indeed, the problem is the unbounded position operator x in the definition of T_0 .

To proceed rigorously, we therefore choose the regularised multiplier

$$\phi := x \cdot \nabla (\xi_n \psi) + \frac{d}{2} \psi, \quad (12)$$

where ξ_n is the cut-off function satisfying, for every $n \in \mathbb{N}^*$, $\xi_n(x) := \xi(x/n)$, where $\xi \in C_0^\infty(\mathbb{R}^d)$ is such that $0 \leq \xi \leq 1$, $\xi(x) = 1$ for every $|x| \leq 1$ and $\xi(x) = 0$ for every $|x| \geq 2$. Then $\phi \in W^{1,2}(\mathbb{R}^d)$ because $\psi \in W^{2,2}(\mathbb{R}^d)$ and the multiplication by x is bounded on the support of ψ_n . Then we get the ultimate identity $\|\nabla \psi\| = 0$ of (10) after taking the limit $n \rightarrow \infty$.

The specialty of the free Hamiltonian H_0 is that the elliptic regularity implies that the eigenfunction ψ belongs to $W^{2,2}(\mathbb{R}^d)$. Without this extra result (which will be particularly the case when we deal with electromagnetic perturbations below), we only have $\psi \in W^{1,2}(\mathbb{R}^d)$. Then an extra regularisation of the multiplier $iT_0\psi$ consists in replacing the gradient in (12) by difference quotients, as originally proposed in our work [5]. Altogether, proceeding rigorously with the regularised multiplier and taking the limits in the right order is rather painful. This is probably the reason why necessary regularisation schemes are usually omitted in the literature, except for the recent work [5].

8 Electromagnetic perturbations

Of course, the absence of eigenvalues of the free Hamiltonian H_0 can be proved more straightforwardly by using the Fourier transform. However, the advantage of the present method based on the virial theorem is that it is much more robust. In particular, the same conjugate operator T_0 applies to electric perturbations of H_0 and its magnetic version enables one to deal with magnetic perturbations of H_0 , too.

Given a scalar function (electric potential) $V : \mathbb{R}^d \rightarrow \mathbb{R}$ and a vector-valued function (mag-

netic potential) $A : \mathbb{R}^d \rightarrow \mathbb{R}^d$, consider the electromagnetic Hamiltonian

$$H_{A,V} := (-i\nabla - A)^2 + V.$$

Under the minimal hypotheses $V \in L^1_{\text{loc}}(\mathbb{R}^d)$ and $A \in L^2_{\text{loc}}(\mathbb{R}^d)$ together with a relative smallness of the negative part of V with respect to the magnetic Laplacian $-\Delta_A := (-i\nabla - A)^2$, the operator $H_{A,V}$ is customarily realised as a self-adjoint operator in $L^2(\mathbb{R}^d)$ with the form domain of $H_{A,V}$ being the magnetic Sobolev space $W^{1,2}_A(\mathbb{R}^d) := \{\psi \in L^2(\mathbb{R}^d) : \nabla_A \psi \in L^2(\mathbb{R}^d)\}$, where $\nabla_A := \nabla - iA$ is the magnetic gradient. Of course, $H_{0,0} = H_0$ is the free Hamiltonian.

Electric perturbations

In the magnetic-free case, one has

$$i[H_{0,V}, T_0] = 2H_0 - x \cdot \nabla V,$$

so the virial identity reads

$$2 \|\nabla \psi\|^2 - \int_{\mathbb{R}^d} x \cdot \nabla V |\psi|^2 = 0 \quad (13)$$

whenever ψ is an eigenfunction of $H_{0,V}$.

Clearly, the pointwise repulsivity condition

$$x \cdot \nabla V \leq 0$$

implies a contradiction, therefore the absence of eigenvalues of $H_{0,V}$. Less restrictively, it is enough to assume the smallness of the positive part $(x \cdot \nabla V)_+$ in the following integral sense: There exists a positive number $a < 2$ such that

$$\int_{\mathbb{R}^d} (x \cdot \nabla V)_+ |\psi|^2 \leq a \int_{\mathbb{R}^d} |\nabla \psi|^2 \quad (14)$$

holds for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Our regularisation scheme described in Section 7 requires the extra regularity condition

$$V \in W^{1,p}_{\text{loc}}(\mathbb{R}^d), \quad (15)$$

where $p = 1$ if $d = 1$, $p > 1$ if $d = 2$ and $p = d/2$ if $d \geq 3$.

The repulsivity condition (14) can be replaced by the following smallness condition, in which case (15) is not needed: There exists a positive number $a < 2/(d+2)$ such that

$$\begin{aligned} \int_{\mathbb{R}^d} |V| |\psi|^2 &\leq a \int_{\mathbb{R}^d} |\nabla \psi|^2, \\ \int_{\mathbb{R}^d} |x|^2 |V|^2 |\psi|^2 &\leq a^2 \int_{\mathbb{R}^d} |\nabla \psi|^2, \end{aligned} \quad (16)$$

hold for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Indeed, it is enough to integrate by parts in the second term on the left-hand side of (13) and use the Schwarz inequality.

Let us summarise the obtained results into the following theorem.

Theorem 1 *Assume (14) with $a < 2$ or (16) with $a < 2/(d+2)$. In the former case assume in addition (15). Then $\sigma_p(H_{0,V}) = \emptyset$.*

This theorem is a very special case of a series of recent results obtained in [6, Thm. 3] and [4, Thm. 3.4]. However, a first rigorous proof of (13) (under alternative regularity hypotheses about V) goes back to Weidmann [11].

Magnetic perturbations

When there is a magnetic field, the conjugate operator (8) should be replaced by its magnetic version

$$T_A := \frac{X \cdot P_A + P_A \cdot X}{2} = -ix \cdot \nabla_A - i\frac{d}{2},$$

where $P_A := -i\nabla_A$ is the magnetic momentum. For simplicity, let us consider purely magnetic perturbations of the free Hamiltonian. Then

$$i[H_{A,0}, T_A] = 2H_{A,0} + (x \cdot B) \cdot P_A + P_A \cdot (x \cdot B),$$

where $B := \nabla A - (\nabla A)^T$ is the magnetic tensor. Consequently, the virial identity reads

$$2 \|\nabla_A \psi\|^2 + 2\Im \int_{\mathbb{R}^d} (x \cdot B) \cdot \psi \overline{\nabla_A \psi} = 0$$

whenever ψ is an eigenfunction of $H_{A,0}$.

Using the Schwarz inequality, we get a contradiction, and therefore the absence of eigenvalues of $H_{A,0}$, provided that the following smallness condition holds: There exists a positive number $a < 1$ such that

$$\int_{\mathbb{R}^d} |x|^2 |B|^2 |\psi|^2 \leq a^2 \int_{\mathbb{R}^d} |\nabla_A \psi|^2 \quad (17)$$

holds for every $\psi \in W^{1,2}_A(\mathbb{R}^d)$. Our regularisation scheme described in Section 7 requires the extra regularity condition

$$A \in W^{1,2p}_{\text{loc}}(\mathbb{R}^d), \quad (18)$$

where p is as below (15).

We have therefore established the following theorem.

Theorem 2 Assume (17) with $a < 1$ and (18). Then $\sigma_p(H_{A,0}) = \emptyset$.

It is important that the fundamental hypothesis (17) is gauge invariant (i.e. it does not depend on the choice of A for a given magnetic field B).

Theorem 2 is a very special case of a series of recent results obtained in [6, Thm. 3] and [4, Thm. 3.4]. The sufficient conditions which guarantee the absence of eigenvalues of $H_{A,V}$ follow from a full electromagnetic virial identity there.

Low versus high dimensions

It is interesting that spectral conclusions can be obtained on the basis of functional inequalities of the type (14), (16) and (17). Because of the criticality of the Laplacian in dimensions $d = 1, 2$, the conditions (16) cannot be satisfied for a non-trivial V in these low dimensions. On the other hand, explicit sufficient conditions to verify the functional inequalities in high dimensions $d \geq 3$ follow by the Hardy inequality. What is more, hypothesis (17) (and other sufficient conditions stated in terms of the magnetic Laplacian ∇_A) is non-void even in dimension $d = 2$ due to the existence of magnetic Hardy inequalities [3].

9 Non-self-adjoint perturbations

There are recent motivations to consider *complex* electromagnetic fields, including quantum mechanics [8]. It is clear already from the manipulations in (4) that the idea based on the virial theorem becomes useless in this case. On the other hand, the method of multipliers turns out to be more flexible.

Let us demonstrate it on the eigenvalue problem for the magnetic-free Hamiltonian

$$H_{0,V}\psi = \lambda\psi, \quad (19)$$

where both the potential V and the eigenvalue λ are allowed to be complex now. We set $\lambda_1 := \Re\lambda$ and $\lambda_2 := \Im\lambda$, and analogously for V . For simplicity, let us assume the following subordination condition: There exists a positive number $b < 1$ such that

$$\int_{\mathbb{R}^d} (|\Re V_-| + |\Im V|) |\psi|^2 \leq b \int_{\mathbb{R}^d} |\nabla\psi|^2 \quad (20)$$

holds for every $\psi \in W^{1,2}(\mathbb{R}^d)$. Then the numerical range of $H_{0,V}$ is contained in the cone $|\lambda_2| \leq \lambda_1$, so it enough to explore the presence of eigenvalues there.

As in Section 3 (and disregarding the necessary regularisation procedures), take an inner product of both sides of (19) with the function $iT_0\psi$, where T_0 is given by (8), and take twice the real part of the obtained identity. This leads to the identity

$$2 \|\nabla\psi\|^2 - \int_{\mathbb{R}^d} x \cdot \nabla V_1 |\psi|^2 - 2\Im(x \cdot \nabla\psi, V_2\psi) = -2\lambda_2 \Im(x \cdot \nabla\psi, \psi) \quad (21)$$

which is a non-self-adjoint counterpart of (13).

The idea of [1] is to compensate the appearance of the imaginary part of the inner product on the second line of (21) with no obvious sign by further identities obtained by using different multipliers. First, taking an inner product of both sides of (19) with the function ψ and taking the real part of the obtained identity, we get

$$\|\nabla\psi\|^2 + \int_{\mathbb{R}^d} V_1 |\psi|^2 = \lambda_1 \|\psi\|^2. \quad (22)$$

Second, taking an inner product of both sides of (19) with the function $|x|\psi$ and taking the real and imaginary part of the obtained identity, we respectively get

$$\begin{aligned} \int_{\mathbb{R}^d} |x| |\nabla\psi|^2 - \frac{d-1}{2} \int_{\mathbb{R}^d} \frac{|\psi|^2}{|x|} + \int_{\mathbb{R}^d} |x| V_1 |\psi|^2 \\ = \lambda_1 \int_{\mathbb{R}^d} |x| |\psi|^2. \end{aligned} \quad (23)$$

and

$$\begin{aligned} \Im \int_{\mathbb{R}^d} \frac{x}{|x|} \cdot \bar{\psi} \nabla\psi + \int_{\mathbb{R}^d} |x| V_2 |\psi|^2 \\ = \lambda_2 \int_{\mathbb{R}^d} |x| |\psi|^2. \end{aligned} \quad (24)$$

By taking the clever sum

$$(21) - (22) + \frac{|\lambda_2|}{\sqrt{\lambda_1}} (23) - 2\sqrt{\lambda_1} \operatorname{sgn}(\lambda_2) (24),$$

we arrive at the ultimate identity

$$\begin{aligned} \|\nabla\psi^-\|^2 + \frac{|\lambda_2|}{\sqrt{\lambda_1}} \int_{\mathbb{R}^d} |x| \left(|\nabla\psi^-|^2 - \frac{d-1}{2} \frac{|\psi^-|^2}{|x|^2} \right) \\ - \int_{\mathbb{R}^d} \frac{x}{|x|} \cdot \nabla(|x|V_1) |\psi|^2 + \frac{|\lambda_2|}{\sqrt{\lambda_1}} \int_{\mathbb{R}^d} |x| V_1 |\psi|^2 \\ - 2\Im \int_{\mathbb{R}^d} V_2 x \cdot \psi^- \overline{\nabla\psi^-} = 0, \end{aligned} \quad (25)$$

where

$$\psi^-(x) := e^{-i\sqrt{\lambda_1} \operatorname{sgn}(\lambda_2) |x|} \psi(x).$$

Various sufficient conditions for the absence of eigenvalues of $H_{0,V}$ can be derived from (25). This has been done in a series of recent papers [4, 6, 7], including the magnetic field and obtaining uniform resolvent estimates.

For instance, let $d \geq 3$, so that the second term on the first line of (25) is non-negative by a weighted Hardy inequality, and assume that the potential V is purely imaginary. Then $H_{0,V}$ has no eigenvalues in the cone $|\lambda_2| \leq \lambda_1$ provided that there exists a positive number $a < 1/2$ such that

$$\int_{\mathbb{R}^d} |x|^2 |\Im V|^2 |\psi|^2 \leq a^2 \int_{\mathbb{R}^d} |\nabla \psi|^2 \quad (26)$$

holds for every $\psi \in W^{1,2}(\mathbb{R}^d)$.

Theorem 3 *Let $d \geq 3$ and $\Re V = 0$. Assume conditions (26) with $a < 1/2$ and (20) with $b < 1$. Then $\sigma_p(H_{0,V}) = \emptyset$.*

10 Relativistic operators

The approach described in the preceding section can be adapted to electromagnetic Schrödinger operators with *matrix-valued* potentials. This has been done in [4], where we also applied the results to establish the absence of eigenvalues of Pauli and Dirac operators.

11 Boundary perturbations

The flexibility of the method of multipliers, particularly due to the developments described in Section 9, enables one to consider elliptic operators constrained to *subdomains* of the Euclidean space. In [5], we developed the method to study spectral properties of the Laplacian in the half-space $\mathbb{R}^{d-1} \times (0, \infty)$, subject to Robin boundary conditions

$$-\frac{\partial \psi}{\partial x_d} + \alpha \psi = 0,$$

where $\alpha : \mathbb{R}^{d-1} \times \{0\} \rightarrow \mathbb{C}$ plays the role of a strongly localised potential. For instance, there are no eigenvalues provided that α is repulsive in the sense that

$$\alpha \geq 0 \quad \text{and} \quad x \cdot \nabla \alpha \leq 0.$$

Moreover, we derive uniform resolvent estimates.

The half-space can be regarded as a degenerate situation of conical domains intensively studied in recent years. In this respect, let us particularly mention the proof of the absence of eigenvalues of the Laplacian in non-convex conical sectors, subject to no specific boundary conditions [2]. On the other hand, it is easy to construct square-integrable solutions to the eigenvalue problem in a half-space.

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